Statistical and Low Temperature Physics (PHYS393)

3. Photons and Phonons

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Learning Aims: You will learn to

State and use the phonon energy distribution. Derive the density of states for phonons. Explain and derive the Debye frequency.

Derive the low and high temperature limits of the phonon heat capacity.

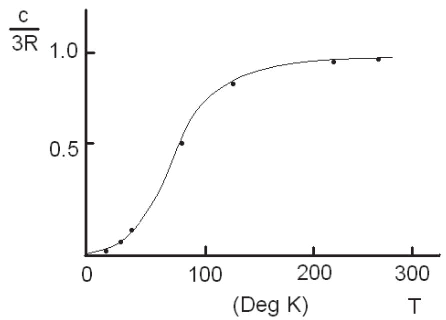
Explain blackbody radiation as a free photon gas. State and use the photon energy distribution. Derive the density of states for photons.

Derive Stefan's law for blackbody radiation.

Phonons

Specific heat capacities of solids

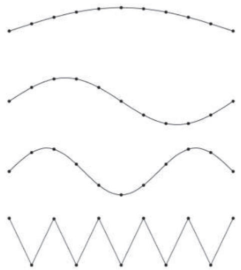
In 1912, Peter Debye, a Dutch physicist working in Germany, produced a theory which predicts the heat capacity of a solid correctly at high and low temperatures.



Atoms vibrating in a solid

In Debye's model, we think of the atoms in a solid as connected by springs. They vibrate in 3D in a complicated way.

The problem can be simplified by treating the vibration as a superposition of waves of different frequencies.



If we suppose that the atoms are fixed at the edge of the solid, the frequency would be quantised. A quantum of this vibration energy is called a phonon.

Quantised thermal waves

We can count the number of states for the phonons, like we did for atoms in an ideal gas, or electrons in a metal.

Unlike electrons, however, the exclusion principle does not apply to phonons.

So each energy state can be occupied by any number of phonons.

Phonon occupation number

The phonon energy distribution is given by

$$n(\varepsilon)d\varepsilon = \frac{g(\varepsilon)d\varepsilon}{\exp(\varepsilon/k_B T) - 1}$$

Next, we need a formula for the density of states $g(\varepsilon)$.

Note that although we have previously used the same symbol $g(\varepsilon)$ for the particle in a 3-D box, the phonon density of states would have a different formula.

density of states for phonons

The vibrations in a solid is described by a wave equation. The solution for the displacement of the atoms ξ , can be given by the same function

$$\xi = \sin k_x x$$

in each of the x, y and z directions. Assuming that the displacements are zero at the edge of the solid, the wavevectors are discretised in the same way:

$$k_x = \frac{n_x \pi}{a}.$$

So the density of states can also be given by the same formula:

$$g(k) = \frac{Vk^2}{2\pi^2}.$$

However, two changes are needed from the way we have used it for the ideal gas and the electrons.

The first change is in the change of variable to energy ϵ.

For atoms or electrons, the energy is

$$\varepsilon = \frac{\hbar^2 k^2}{2m}.$$

For vibrations, the energy is given by by the same formula as for photons:

$$\varepsilon = \hbar\omega,$$

where ω is the angular frequency $2\pi f$ and f is the frequency. ω is in turn related to k by

$$v = \frac{\omega}{k},$$

where v is the velocity.

The variable of angular frequency ω is often used instead of energy ε. For the change of variable, we then use

$$\omega = vk.$$

We can now do the change of variable using

$$g(\omega)d\omega = g(k)dk.$$

Substituting

$$g(k) = \frac{Vk^2}{2\pi^2},$$

we get the density of states in ω:

$$g(\omega) = \frac{V\omega^2}{2\pi^2 v^3}.$$

About polarisation

The second change is the related to the polarisation. Recall that for electrons, we have to multiply by 2 because of the 2 spin states.

For vibration, a state is a particular frequency, for a particular set of wavevectors (k_x, k_y, k_z).

Each state correspond to a wave, and a wave in a solid can have 2 transverse polarisations, and 1 longitudinal polarisation.

So we have to multiply by 3 to get the correct density of state:

$$g(\omega)d\omega = 3 \times \frac{V\omega^2 d\omega}{2\pi^2 v^3}$$

The Debye Frequency

There is one more practical point to note. In a solid, there is a limit to the highest phonon frequency.

This is related to the fact that the wavelength cannot possibly be shorter than the distance between atoms.

Let this highest frequency be ω_D.

In a solid with N identical atoms, there are $3N$ energy states, or normal modes. This is when we count every possible frequency, and every possible "direction of vibration" for each frequency.

This can be proven mathematically, but we shall skip that. We can find ω_D by integrating the density of states:

$$\int_0^{\omega_D} g(\omega)d\omega = \int_0^{\omega_D} \frac{3V\omega^2 d\omega}{2\pi^2 v^3} = 3N$$

This equation

$$\int_0^{\omega_D} g(\omega)d\omega = \int_0^{\omega_D} \frac{3V\omega^2 d\omega}{2\pi^2 v^3} = 3N$$

can then be solved to find the Debye frequency. Integrating gives

$$\frac{V\omega_D^3}{2\pi^2 v^3} = 3N$$

Solving for ω_D gives the Debye frequency:

$$\omega_D = \left(\frac{6N\pi^2 v^3}{V}\right)^{1/3}$$

As we have shown earlier, the distribution of phonons is given by

$$n(\varepsilon)d\varepsilon = \frac{g(\varepsilon)d\varepsilon}{\exp(\varepsilon/k_B T) - 1}$$

We shall express this in terms of frequency ω as well. The phonon energy ε is given by

$$\varepsilon = \hbar\omega.$$

This comes from assuming that the atoms vibrate in a harmonic potential, so that the energy is quantised in steps of $\hbar\omega$.

In terms of the frequency ω, the phonon distribution is then given by

$$n(\omega)d\omega = \frac{g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

The phonon distribution is given by

$$n(\omega)d\omega = \frac{g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

We can multiply by $\hbar\omega$ to get the energy at this frequency interval:

$$\hbar\omega n(\omega)d\omega = \frac{g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

The total energy is then

$$U = \int_0^{\omega_D} \hbar\omega n(\omega)d\omega = \int_0^{\omega_D} \frac{\hbar\omega g(\omega)d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

We have found earlier that the density of states is:

$$g(\omega) = 3 \times \frac{V\omega^2}{2\pi^2 v^3}.$$

Substituting into the integral for the total energy above ...

We get:

$$U = \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} \frac{\omega^3 d\omega}{\exp(\hbar\omega/k_B T) - 1}$$

At low temperature, it can be shown that this is proportional to T^4. This would imply that the heat capacity C is proportional to T^3. (This has been mentioned in the topic on the specific heat of electrons in metal.)

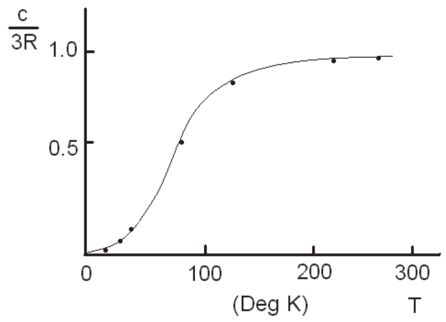
The T^4 behaviour is derived by making the substitution

$$x = \hbar\omega/k_B T.$$

As T gets small, x becomes large. So the upper limit is substituted with ∞. Then using the formula on the last page of these notes, it can be integrated to give the T^4 behaviour.

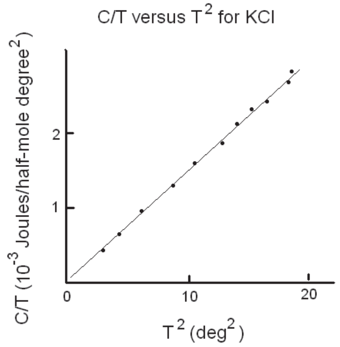
At high temperatures, the heat capacity tends to $3Nk_B$.

In 1912, Debye measured the high temperature behaviour of copper. This picture shows a sketch of the molar heat capacity of copper that he measured.



He showed that the heat capacity did tend to $3Nk_B$, as he had predicted.

In 1953, at Purdue University, Keesom and Pearlman measured the low temperature behaviour of potassium chloride. This picture is a sketch of the results.



As predicted by Debye, the heat capacity was indeed proportional to T^3.

Photons

An object at a certain temperature would emit and absorb electromagnetic radiation. The higher the temperature, the higher the average frequency of the radiation emitted.

When an object gets very hot, this frequency can go as high as visible light. For example, the temperature of a volcano lava flow can be estimated by observing its color. The result agrees well with the measured temperatures of lava flows at about 1,000 to 1,200 deg C.

http://en.wikipedia.org/wiki/Black_body

The amount of radiation emitted depends on the nature of the object - its colour, whether it is smooth or rough, etc.

We are particularly interested in an ideal black body, one that absorbs all the radiation that falls on it. The reason is that the radiation emitted by such a body does not depend on its nature at all.

No real material can do this. Soot is about the best, absorbing all but 3%.

In 1859 Gustav Kirchhoff had a good idea: "a small hole in the side of a large box is an excellent absorber, since any radiation that goes through the hole bounces around inside, a lot getting absorbed on each bounce, and has little chance of ever getting out again."

(http://galileo.phys.virginia.edu/classes/252/black_body_radiation.html)

The energy of the absorbed radiation reaches equilibrium among different frequencies in the cavity. This results in a characteristic spectrum that would be emitted again through the hole.

We can derive a formula for the spectrum of black body radiation by considering the energies of a free photon gas in a box (following Kirchhoff's idea).

Photons arise from oscillations in electromagnetic fields, which is also governed by a wave equation.

The same ideas for phonons can be used, leading to the same density of states:

$$g(\omega) = \frac{V\omega^2}{2\pi^2 c^3},$$

where the speed v is now the speed of light c. This is the formula before considering polarisations.

Like phonons, the photon number is not fixed. We get few photons when the box is cold, and more photons when it is hot.

Unlike phonons, there is no upper limit to the frequency (no Debye frequency). The wavelength in a solid cannot be shorter than the distance between atoms. The electromagnetic wave in a box has no such limit.

Finally, phonons in a solid can have 3 polarisations: 2 transverse and 1 longitudinal (like sound). Photons can only have 2: both transverse (e.g. light).

Recall that for phonons, the density of states is give by:

$$g(\omega)d\omega = 3 \times \frac{V\omega^2 d\omega}{2\pi^2 v^3}$$

where the factor of 3 comes from the 3 polarisations of a phonon, 2 transverse and 1 longitudinal.

Since photons only have 2 polarisations, both transverse, the 3 should be replaced by a 2:

$$g(\omega)d\omega = 2 \times \frac{V\omega^2 d\omega}{2\pi^2 c^3}$$

where the sound speed v is replaced by light speed c.

Distribution of photon number

Like phonons, each energy state can be occupied by any number of photons.

So it obeys Bose-Einstein statistics.

The number density is therefore given by the same formula:

$$n(\epsilon)d\epsilon = \frac{g(\epsilon)d\epsilon}{\exp(\varepsilon/k_B T) - 1}$$

So the number of photons in a given frequency interval is

$$n(\omega)d\omega = 2 \times \frac{V\omega^2 d\omega}{2\pi^2 c^3} \times \frac{d\omega}{\exp(\hbar\omega/k_B T) - 1}$$

Distribution of photon energy

The energy of a photon is $\hbar\omega$. The energy in the frequency interval $d\omega$ is then

$$\hbar\omega n(\omega)d\omega = 2 \times \hbar\omega \times \frac{V\omega^2 d\omega}{2\pi^2 c^3} \times \frac{d\omega}{\exp(\hbar\omega/k_B T) - 1}$$

The energy is given by:

$$u(\omega) = \hbar\omega n(\omega) = \frac{V\hbar\omega^3}{\pi^2 c^3} \frac{1}{\exp(\hbar\omega/k_B T) - 1}.$$

This is also formula for the spectrum, and is called Planck's law for black body radiation. Integrating gives the total energy:

$$U = \frac{\pi^2 V k_B^4}{15\hbar^3 c^3} T^4$$

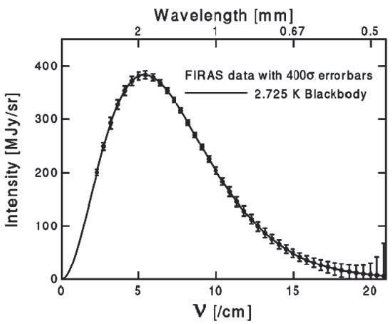
It can be shown that this leads to Stefan's law of radiation:

$$\eta = \sigma T^4$$

for radiation emitted by an object at a temperature T.

Example

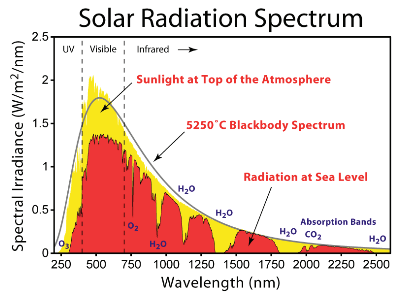
The cosmic microwave background is an example of blackbody radiation. The spectrum has been measured. Planck's radiation formula is then fitted to the spectrum.



Using a temperature value of 2.74 K in the formula was found to fit the measurement well. This tells us that deep space has a temperature of 2.74 K.

Example

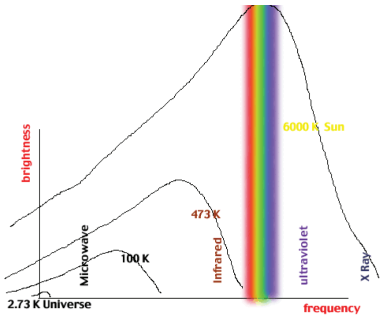
In the same way, Planck's formula may be fitted to the sun's spectrum.



(http://en.wikipedia.org/wiki/Sunlight)

A 5800 K temperature gives a reasonable fit. However, part of the fitted curve deviates from measured data. This could be due to absorption by atmosphere, or emission from other sources.

The radiation spectrum of a higher temperature object peak at higher frequency.



(http://www.launc.tased.edu.au/online/sciences/physics/blackbody1.html)

For example, human emit radiation with the peak in the infrared wavelength 9.3 μm. A hot plate at 400 $^\circ$C has a peak at 4.3 μm, with a bit in visible red. That is why it looks red hot.

Worked Examples

Example 1

(i) Write down the integral expression for the total energy of phonons in a solid. Write down the formula for Debye frequency. Define all symbols.

(ii) Make the substitution $x = \hbar\omega/k_B T$ where ω is the angular frequency and T is the temperature. Find the expression for the integral for at the low temperature limit.

(iii) Integrate to find the total energy. Show that phonon heat capacity is proportional to T^3 at the low temperatures.

Solutions

(i) Expression for total energy is

$$U = \int_0^{\omega_D} \frac{\hbar\omega g(\omega) d\omega}{\exp(\hbar\omega/k_B T) - 1}.$$

where ω_D is the Debye frequency, ω the angular frequency, $g(\omega)$ the density of states and T the temperature.

Formula for Debye frequency is

$$\omega_D = \left(\frac{6N\pi^2 v^3}{V}\right)^{1/3}$$

where N is total number of atoms, v is speed of sound and V is volume of solid.

(ii) Rearrange:

$$\omega = \frac{k_B T x}{\hbar}.$$

For the upper limit, ω_D, of the integral, let the corresponding x be x_D. So

$$x_D = \frac{\hbar\omega_D}{k_B T}.$$

Density of states of phonons is:

$$g(\omega)d\omega = \frac{3V\omega^2}{2\pi^2 v^3}d\omega.$$

Transforming to x variable:

$$g(x)dx = \frac{3V}{2\pi^2 v^3}\left(\frac{k_B T x}{\hbar}\right)^2 \frac{k_B T}{\hbar}dx.$$

Regrouping terms:

$$g(x)dx = \frac{3Vk_B^3T^3}{2\pi^2 v^3\hbar^3}x^2 dx.$$

Combining the above into the integral:

$$U = \int_0^{x_D} k_B T x \times \frac{g(x)dx}{\exp(x) - 1},$$

Substitute the expression for $g(x)dx$:

$$U = \int_0^{x_D} k_B T x \times \frac{3Vk_B^3T^3}{2\pi^2 v^3\hbar^3} \times \frac{x^2 dx}{e^x - 1},$$

Factor terms that do not depend on x:

$$U = \frac{3Vk_B^4T^4}{2\pi^2 v^3\hbar^3} \times \int_0^{x_D} \frac{x^3 dx}{e^x - 1}.$$

If T goes to zero,

$$x_D = \frac{\hbar\omega_D}{k_B T}$$

goes to infinity. So at the low temperature limit,

$$U = \frac{3Vk_B^4T^4}{2\pi^2 v^3\hbar^3} \times \int_0^{\infty} \frac{x^3 dx}{e^x - 1}.$$

(iii) To find the total energy, we use the result

$$\int_0^{\infty} \frac{x^3}{e^x - 1}dx = \frac{\pi^4}{15}.$$

Substitute into the low temperature limit above, we finally get

$$U = \frac{3Vk_B^4T^4}{2\pi^2 v^3\hbar^3} \times \frac{\pi^4}{15}.$$

Differentiating with respect to T, we get the heat capacity:

$$C = \frac{2Vk_B^4\pi^4}{5\pi^2 v^3\hbar^3} \times T^3,$$

which is proportional to T^3.

Example 2

(i) Write down the integral expression for the total energy of photons in a box.

(ii) Make the substitution $x = \hbar\omega/k_B T$ where ω is the angular frequency and T is the temperature. Integrate to find the total energy.

(iii) Stefan's law gives the power per unit area coming out in all directions through a hole on the box ('per unit area' referring to area of the hole). Assuming that radiation is only emitted in the direction normal to the area, find an approximate formula for Stefan's law. Why is this approximate?

Solution

(i) The expression for total energy is

$$U = \int_0^\infty \frac{V\hbar\omega^3}{\pi^2 c^3} \frac{1}{\exp(\hbar\omega/k_B T) - 1} d\omega.$$

where V is volume and T is temperature.

(ii) Rearranging,

$$\omega = \frac{k_B T}{\hbar} x.$$

Substituting into the integral:

$$U = \int_0^\infty \frac{V\hbar}{\pi^2 c^3} \times \left(\frac{k_B T}{\hbar} x\right)^3 \times \frac{1}{\exp(x) - 1} \times \frac{k_B T}{\hbar} dx.$$

The limits remain the same since x and ω are proportional. Regrouping,

$$U = \frac{V k_B^4 T^4}{\pi^2 c^3 \hbar^3} \times \int_0^\infty \frac{x^3}{e^x - 1} dx.$$

Using this result:

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}.$$

we find

$$U = \frac{V k_B^4 T^4}{\pi^2 c^3 \hbar^3} \times \frac{\pi^4}{15}.$$

(iii) Recall the formula for water flowing through a pipe:

$$\text{mass per second} = \text{density} \times \text{area} \times \text{velocity.}$$

Instead of mass, we have energy here. So the formula becomes

$$\text{power} = \text{energy density} \times \text{area} \times \text{speed of light.}$$

For Stefan's law, we want the intensity η:

$$\frac{\text{power}}{\text{area}} = \text{energy density} \times \text{speed of light.}$$

The energy density is energy / volume $= U/V$. So we have

$$\eta = \frac{Uc}{V}.$$

Substituting the above result for U, we get

$$\eta = \frac{c}{V} \times \frac{V k_B^4 T^4}{\pi^2 c^3 \hbar^3} \times \frac{\pi^4}{15}.$$

Simpifying, we have an approximate Stefan's law:

$$\eta = \frac{\pi^4 k_B^4}{15\pi^2 c^2 \hbar^3} \times T^4.$$

This is approximate because radiation can really come out in all directions. We have not taken this into account.

Learning Outcome: You should be able to

State and use the phonon energy distribution. Derive the density of states for phonons. Explain and derive the Debye frequency.

Derive the low and high temperature limits of the phonon heat capacity.

Explain blackbody radiation as a free photon gas. State and use the photon energy distribution. Derive the density of states for photons.

Derive Stefan's law for blackbody radiation.

Useful Integrals

For Debye model, to find heat capacity at low temperature; and for black body radiation, to find Stefan's law:

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}.$$

For liquid helium-4, later in the course:-

to find condensation temperature of Bose Einstein condensate:

$$\int_0^\infty \frac{x^{1/2}}{e^x - 1} dx = 2.315$$

to the find heat capacity:

$$\int_0^\infty \frac{x^{3/2}}{e^x - 1} dx = 1.783$$